

Ethanone, 1-(3-hydroxyphenyl)-
121-71-1 | DTXSID5059533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.16

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 7.47e-01

Nearest Neighbors from the Training Set

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

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tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

Image not found

Paraldehyde

Measured: 3.02

Predicted: 2.77

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2,2-Dimethylpropane-1,3-diol

Measured: 4.68

Predicted: 4.44